Predictive Models for Semiconductor Device Design and Processing (TCAD Challenges and Solutions)

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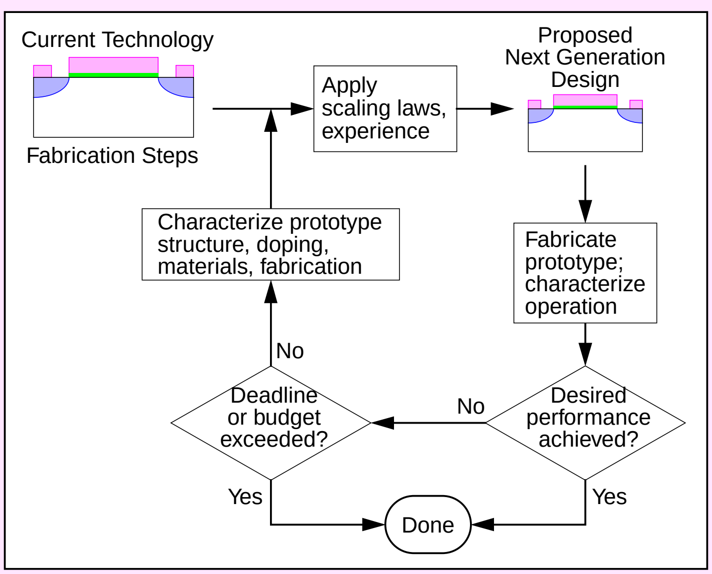
Outline

- **Background**
- **Device and Process Physics**
- **TCAD Software Development**
- **Computational Power**
- **TCAD Software Verification**

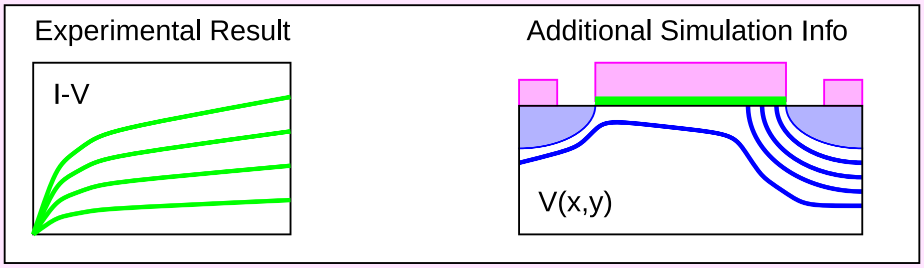
(http://www.ipt.arc.nasa.gov)

Traditional Approach to Device R&D: Scaling Laws/Experimental Iteration



Advantages of TCAD Over Scaling Laws/Experimental Iteration

- Much less expensive
- Investigation of innovative ideas (e.g., quantum devices)
- View of internal processes
- Investigation of individual physical effects
- Ultimate control of materials, structures, environment, tests, etc.



Why is TCAD not the focus in device technology advancement?

TCAD Tools: Where We Stand

Existing TCAD capabilities:

- 3-D process and device simulation
- Intuitive graphical user interface (GUI)
- High-quality graphical output (1-D, 2-D, 3-D, transient)
- Optimized for large computations
- Coupling of simulation tools

Remaining TCAD challenges:

- Limited variety, flexibility, hierarchy, interaction of models
- Code enhancements costly, controlled by developer
- Needed computations are huge
- Little accountability in comparison to experiment

Challenge 1: Process and Device Physics

Process Physics:

- Major process/material changes (e.g., copper, SOI)
- Bulk physics inadequate: poly-crystal grain, atomic physics
- Process history effects (e.g., damage, passivation)
- Cross-wafer/cross-reactor variation

Device Physics:

- Small-geometry/high-field effects:
  - hot electron transport, punch-through, avalanche multiplication, drain-induced barrier lowering, oxide and junction breakdown, leakage currents, grain-size effects, discrete dopant effects, etc.
- Microwave effects
- Quantum effects:
  - gate oxide tunneling, inversion layer quantization, quantum transport, transconductance degradation, etc.

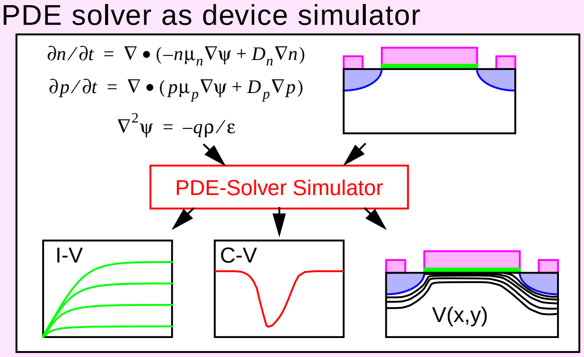
Challenge 1: Solution

Challenge: Conventional approach to implementing P&D models can’t keep up with physics

Requirements:

- variety: models must span relevant physics
- flexibility: ability to modify models as desired
- hierarchy: encapsulate physics at different length/time scales
- interaction: coupling of models in adjoining regions

Solution: Use PDE solver as device simulator



PDE Models for Electronic Devices

Complexity, Comp. Cost	Classical	Quantum-Corrected	Quantum
Low	Drift-diffusion	Density-gradient	Schrödinger, Transfer matrix
Moderate	Energy balance, Hydrodynamic	Quantum EB, Quantum HD	Density matrix, Wigner function
High	Boltzmann transport equation	Quantum Boltz-mann equation	Green's functions
Microwave, Optoelectronic	Substitute Maxwell's equations for Poisson equation		

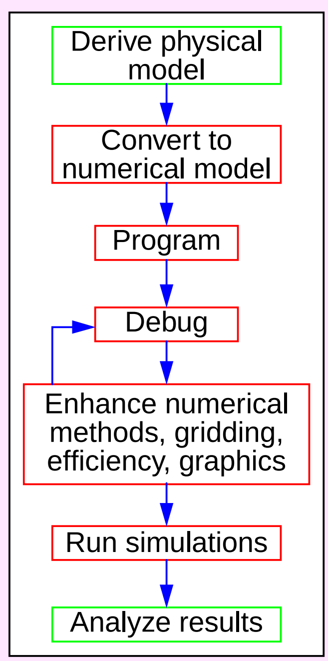
Challenge 2: TCAD Software Development

Developing TCAD tools is difficult:

- Distance to results analysis is long
- Few coding short-cuts are available
- Difficult for experts to "plug in"
- Little collaboration outside of groups
- No standard for tool interaction

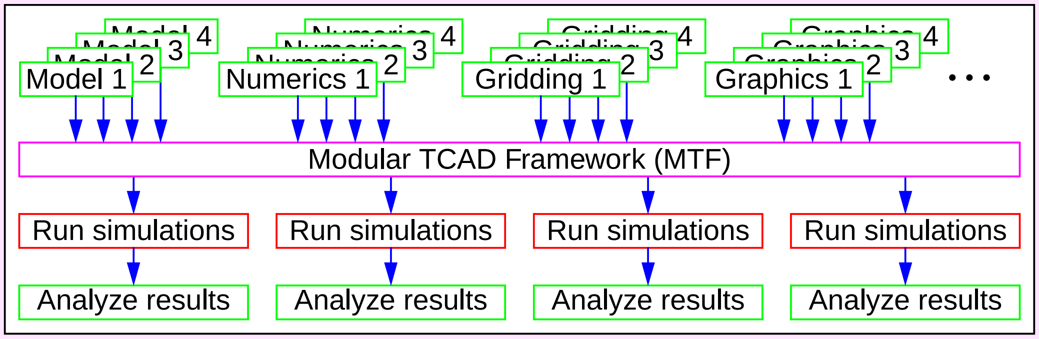
TCAD tools are "stupid"

- Don't learn from experience
- Rudimentary interaction with users



Challenge 2: Solution

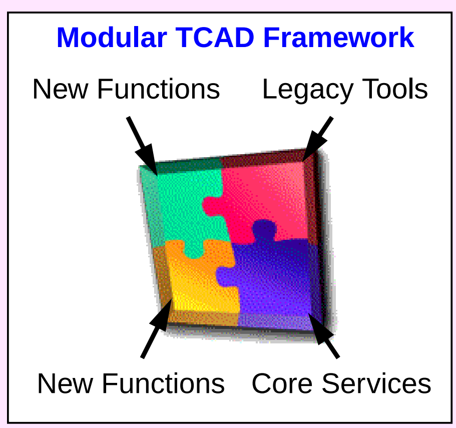
Modular TCAD framework (MTF) as development platform



- Short distance from concept to results
- Encourages collaboration, code sharing
- Experts can “plug in” their expertise
- Code not controlled by one developer/company
- Tool interaction (e.g., process, device) is standardized
- Intelligent features can be implemented

MTF: Tool Developer Interests

- Plenty of work
- Preserve intellectual property
- Easy to plug into
- New facilities for existing tools
- Collaboration-at-a-distance
- Attractive to users

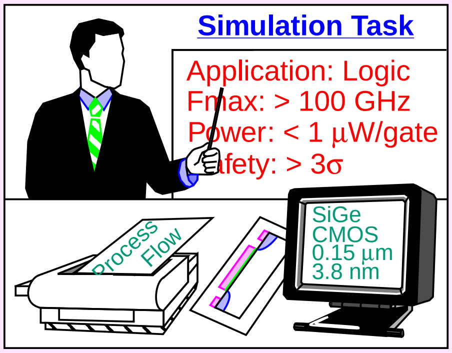


Additional tool vendor interests:

- Protect existing products and customer base
- Add value that people will pay for

MTF: User Interests

- Greater functionality
- Better accuracy
- Fewer bugs
- Better ease of use
- More flexibility to modify models, devices, tests
- Bigger problems, more robustness, faster execution
- Platform independence
- Better technical support
- Low initial investment
- High-level functionality using "Artificial intelligence"



MTF: Artificial Intelligence

Expert System Description	Implementation	Rank
Speech recognition	Commercial	3
Natural language and math expression interpretation	Commercial	2
Estimation of device structure or operation	Data mining ES	1
Estimation of computational resources needed	Data mining ES	1
Selection of optimal physical model(s)	Data mining ES	2
Selection of optimal gridding, numerics, solution algorithms	Data mining ES	2
Correction of non-convergence, excess error, device malfunction	Rule-based ES	2
Interactive visualization	Commercial/NASA	1
Gesture recognition	Commercial/NASA	3
Extraction of default and user-defined results/parameters	Rule-based ES	3
Optimization of device according to specified constraints	Rule-based ES	1
Default and user-specified interaction between tools	Rule-based ES	1
Analyze discrepancies between experiment, simulation	Rule-based ES	2
Tune physical model and RSMs using experimental data	Rule-based ES	3
Apply context-sensitive user and default preferences	Rule-based ES	3

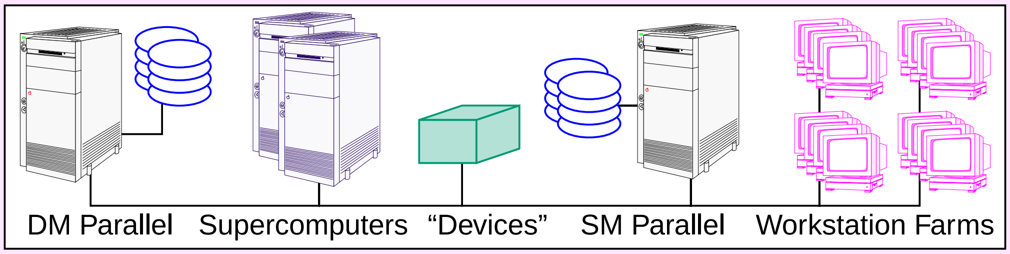
Note: ES = expert system; Rank = relative importance

Challenge 3: Computational Power

Observations:

- Many TCAD computations of interest beyond feasibility
- Uncountable CPU cycles are wasted “bit-flips”

Solution: Link massive numbers of heterogeneous, distributed compute resources as virtual supercomputer; provide simple access

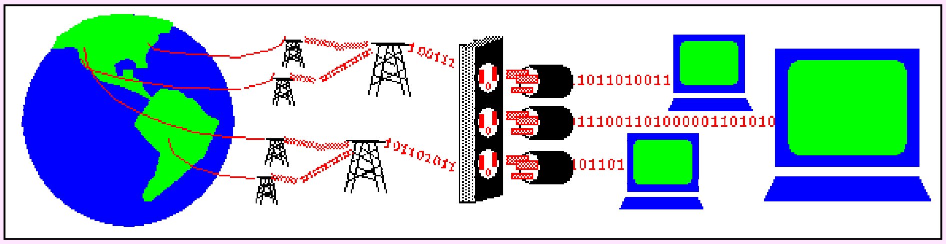


Projects underway:

- NSF: NPACI
- NASA: Information Power Grid (IPG)

IPG: Benefits/Goals

- De-couple computational resources from intellectual resources
- Minimize cost of supercomputing
- Provide transparent access
- Enable collaboration-at-a-distance
- Provide web interface for users, developers

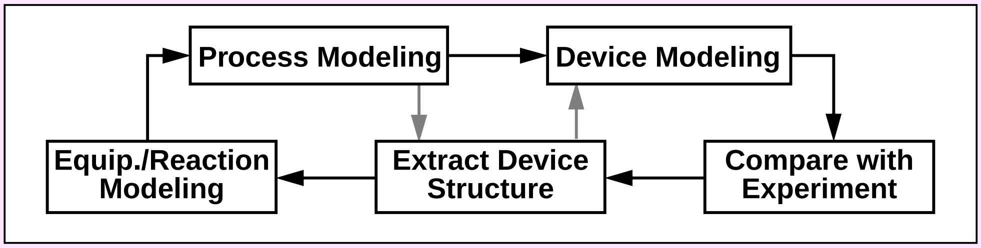


Challenge 4: TCAD Software Verification

Little accountability in TCAD for simulation error

- Process tool developer/user blames device simulation
- Device tool developer/user blames device structure
- Both blame inaccurate measurements/fabrication

Solution: Closed-Loop Device R&D:



Only as good as weakest link!

Activities of NASA Ames NanoScience IPT

Semiconductor Device Modeling

- Semiclassical Electronics (PDE solver approach)
- Nanostructure Quantum Electronics
- Atomic Chain Electronics
- Quantum Optoelectronics

Equipment/Reactor Modeling

- Virtual reactors (including PDE solver approach)
- Microtopography evolution
- Coupling of above
- Gas composition sensor on a chip

Computational Chemistry

- Reaction pathways, rates, kinetics database

Web-Based Process and Device Modeling

Summary

Consequences of lagging TCAD capabilities

- Semiconductor R&D much more expensive
- Evolutionary advancement delayed
- Innovative advancement very difficult

TCAD Challenges and Solutions

- TCAD physics complicated, changing: PDE solver approach
- TCAD software development is difficult: TCAD framework
- Huge computational power needed: Information Power Grid
- Little TCAD verification: Close the loop, improve fab hardware